The NIST Chemistry WebBook

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The NIST Chemistry WebBook (http://webbook.nist.gov) is site on the Internet that provides physical property data to engineers, scientists, and educators worldwide. The site is part of the NIST Standard Reference Data Program and includes data compiled by NIST and outside researchers.

The site is designed to provide access to data in a convenient and timely manner. Where appropriate, citations to the literature are provided along with the data. In many cases, the data are accompanied by comments and auxiliary data from the researchers who collected the data.

A wide range of physical and chemical property data is available from the site. Thermodynamic data include properties for single phases, phase transitions, and reactions. Several large databases of ion energetics data are incorporated in the site, including data for simple ions and ion clusters. Spectral data include gas and condensed phase IR spectra, UV/Vis spectra, and mass spectra. Vibrational and electronic spectra are available for a number of transient and stable species. The site also includes a collection of constants of diatomic molecules and a collection of Henry's law constants. Where appropriate, applets are provided to allow users to view data graphically. In many cases, spectra are available as JCMAP-DX or SVGfiles.

The site also includes two special tools. The first is a set of interactive physical property models developed by the NIST Boulder Labs. These models provide thermodynamic and transport property data for a number of industrially important fluids. The second tool is a group-additivity based estimator for gas phase thermodynamic properties.

The estimator lists all the increments and corrections used in the generation of estimates, so users can clearly see how the estimates were computed. This demonstration will illustrate some of the features of the site and provide tips for efficient usage of the site.